Supplementary Material to the article “Atypical violation of Stokes-Einstein relation in a dense binary Lennard-Jones mixture”

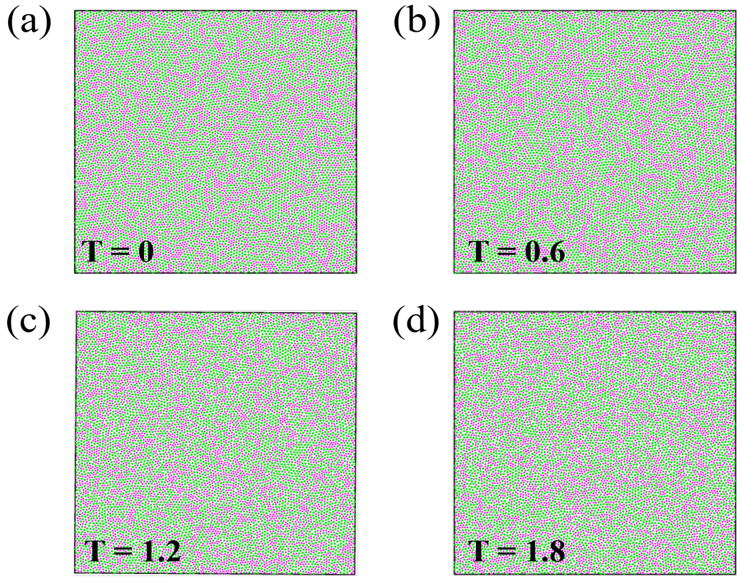

Figure S1: Figures show the cofiguration of the particles for $\alpha = 0.8$ from freezing temperature to melting state. In all the cases green colour represents A-type particles and magenta colour reresents B-type particles.

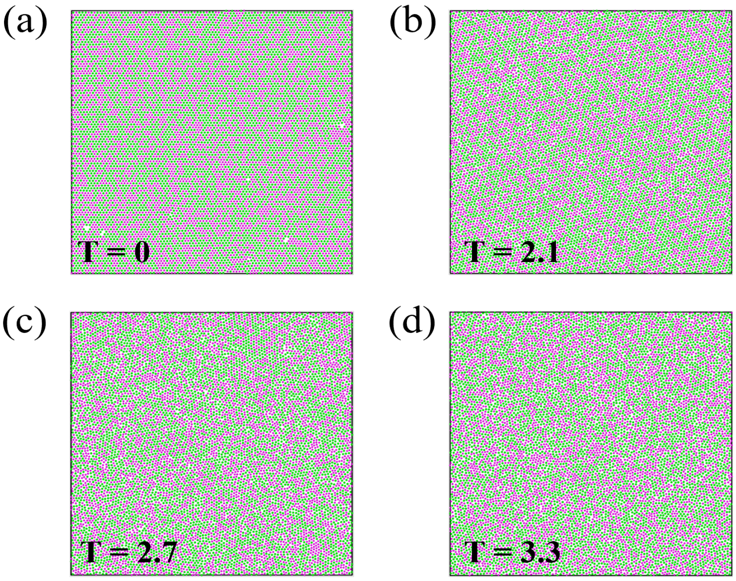

Figure S2: Configuration of the big (green sphere) and small (magenta sphere) particles for $\alpha = 0.9$ at temperatures $T = 0$ to $T = 3.3$ in the figures (a) to (d) respectively.

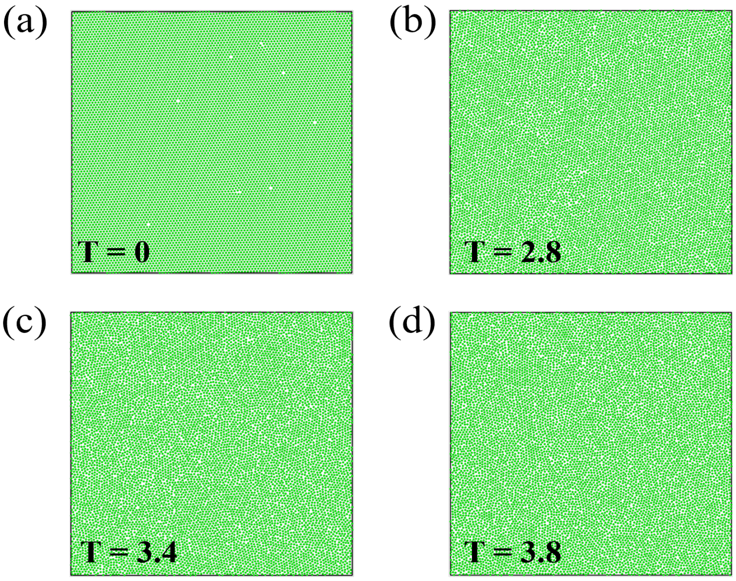

Figure S3: Particle configuration for $\alpha = 1.0$ (one-component system) at temperatures $T = 0, 2.8, 3.4,$ and $T = 3.8$ respectively.

Figures S1 S2, and S3 represents the snapshots of the particle configurations at freezing state

($T = 0$) to the liquid state for the size-ratio $\alpha = 0.8, 0.9$, and 1.0 respectively. These snapshots clearly illustrate that in each case, at freezing temperature, the particles exhibit an ordered arrangement, whereas in the liquid state, they are randomly distributed within the two-dimensional box.

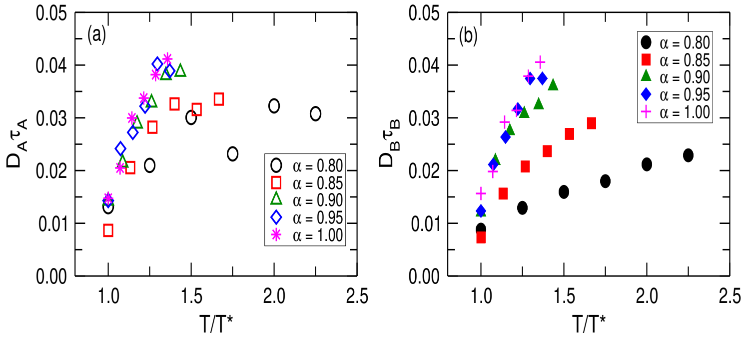

Figure S4: Figure shows $D_S\tau_S$ vs. T/T^* for (a) big and (b) small particles, respectively.

Here, the figure S4 illustrates the product ($D_S\tau_S$) as a function of temperature (T/T^*) for big ($D_A\tau_A$) and small ($D_B\tau_B$) particles in a binary Lennard-Jones (LJ) system with varying size ratios (α). These results highlight the distinct temperature dependence of $D_S\tau_S$ for big and small particles, emphasizing the impact of particle size and interaction parameters on diffusion behaviour. In figure S4(a), for big paricles, the product $D_A\tau_A$ increases non-linerly with the increase in T/T^*. This product also increases with rise in T/T^* but the trend differs as those of the big particles (as shown in the figure S4(b) showing a greater sensitivity to the varying size-ratio. This trend is also found when the product $D_S\tau_S$ is plotted as a function of T. Hence there is no distinct universality in the results after scaling with transition temperature as observed by Khrapak et al.[1] , in which they have used the freezing density scaling and freezing temperature scaling to estimate the transport properties of simple liquids across their phase diagrams.

1. S. A. Khrapak and A. G. Khrapak. Freezing temperature and density scaling of transport coefficients. *J. Phys. Chem. Lett.*, 13(12):2674–2678, 2022.